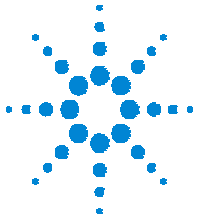
GC/FID & GC/MS RTL Flavor Databases

User Contributed by

Agilent Technologies

Wilmington, Delaware, USA

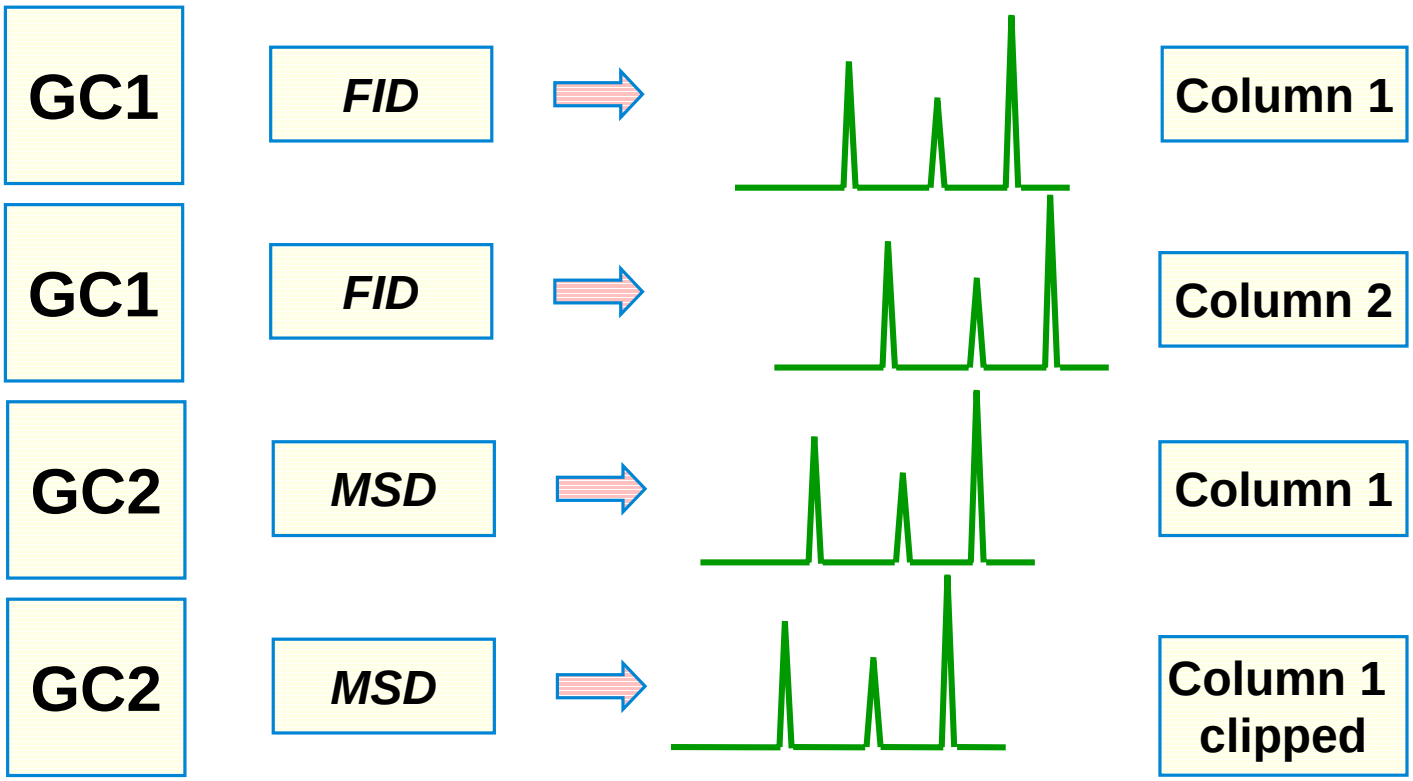


Agilent Technologies

Innovating the HP Way

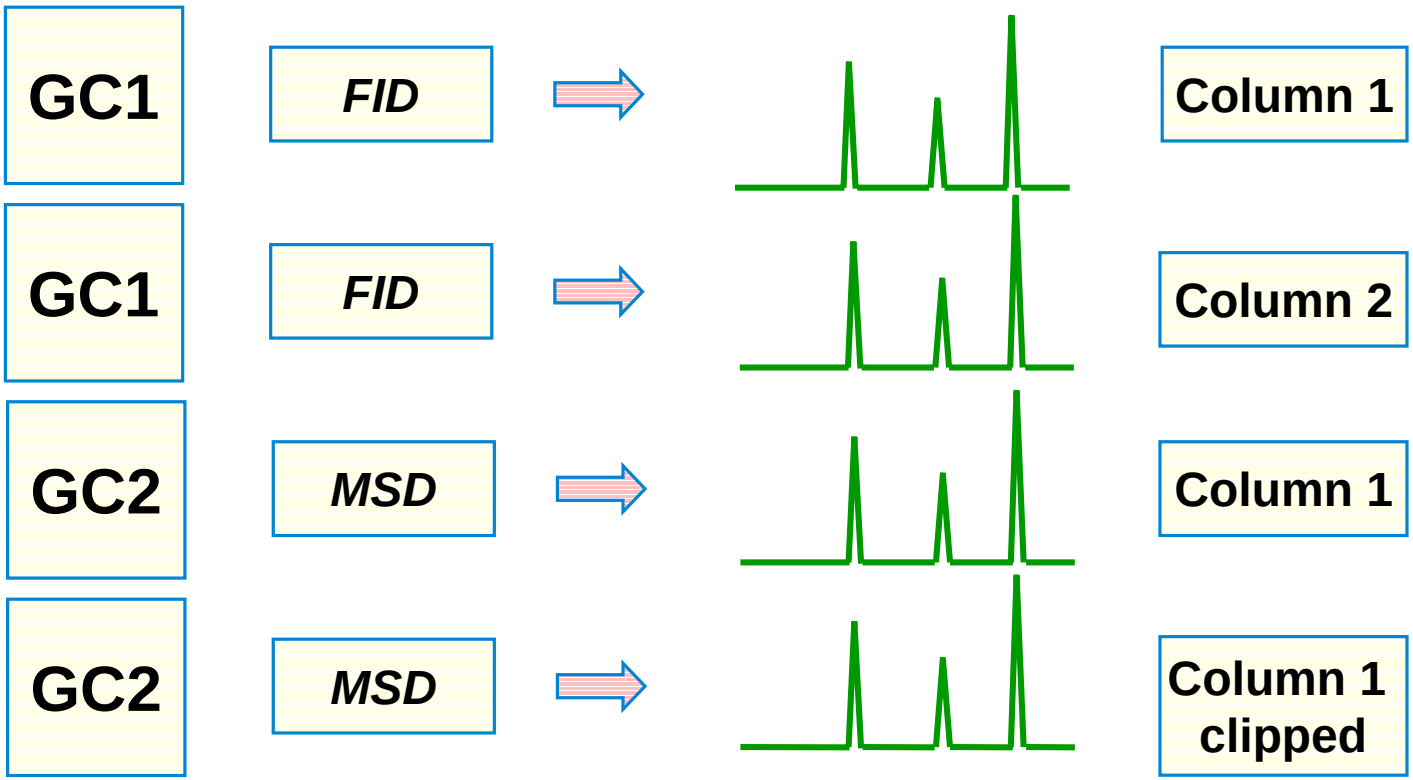
Why Use Retention Time Locking ?

Retention times shift with column maintenance or detector



Using Retention Time Locking

Retention times are reproducible to 0.030 min or better



Benefits of RTL

- Pattern profiles can be superimposed
- Quantitation database times stay the same
- SIM group switching times stay the same
- Integration event times stay the same
- Troubleshooting simplified
- Comparing data from other testing facilities
- GC/FID database can search on retention time instead of retention index
- GC/MS Screener database can search on retention time as a qualifier

Database Development

- Developed by
  - Research Institute for Chromatography, Kortrijk, Belgium
  - Quest International, Naarden, The Netherlands
  - Laboratory of Organic Chemistry, University of Gent, Belgium
  - In cooperation with Agilent Technologies
- All retention time and spectral data collected on Agilent GC/FID and GC/MSD systems

There are 2 GC/MS Databases

- **Retention Time Locked Screener Database**
  - **Flavor2.scd**
  - **409 compounds with precise retention times**
  - **target ion and up to 3 qualifier ions**
- **Mass Spectral Library**
  - **Flavor2.L**
  - **GC/MS Spectra for the 409 compounds**
- **RTLocked to n-pentadecane at 27.500 min**
  - **30 m x 250 µm x 0.25 µm HP-5MS, 19091S-433**

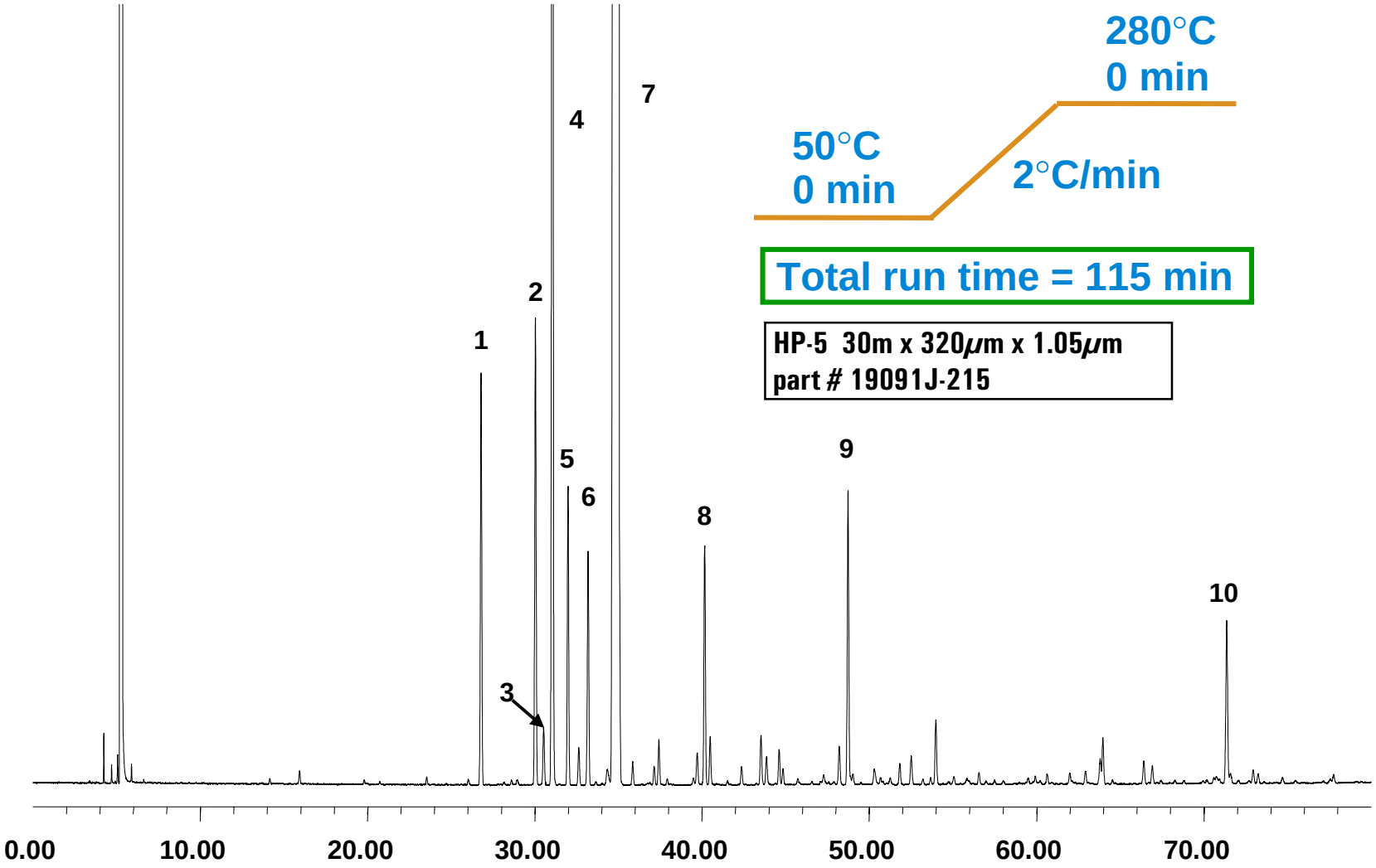
There is also 1 GC/FID Database

- Retention Time Locked Database
  - **Flavfid.rtt**
  - **Same 409 compounds as the GC/MS databases**
  - **precise retention times**
- RTLocked to n-pentadecane at 70.000 min
  - **50 m x 320 µm x 1.05 µm HP-5, 19091J-215**

Using the GC/FID Flavor Database

- Flavfid.rtt is copied to the C:\Hpchem\Rtl folder
- The GC/FID system is retention time locked and an RTL method is established
- Samples are run using the RTL method
- Sample datafile is analyzed using Flavfid.rtt
  - interactively with the RTSearch menu item
  - automatically with the user contributed macro Autosrch.mac
- Results can be saved or printed

Spanish Orange Oil - RTLocked GC/FID



Search Results - Spanish Orange Oil

Peak number	GC-FID t_R (min)	t_R identification	GC-MS t_R (min)	MS + t_R identification
1	26.793	α-pinene	5.172	α-pinene
2	30.042	1-octen-3-ol 3-(methylthio)-1-propanol sabinene	6.181	sabinene
3	30.539	hexanoic acid β-pinene 6-methyl-5-hepten-2-one	6.282	β-pinene
4	31.053	2-octanone myrcene furfuryl acetate	6.658	myrcene
5	31.987	octanal	6.987	octanal
6	33.190	trans 2-hexenoic acid Δ-3-carene	7.267	Δ-3-carene
7	35.001	limonene benzylalcohol ocimene	8.130	limonene

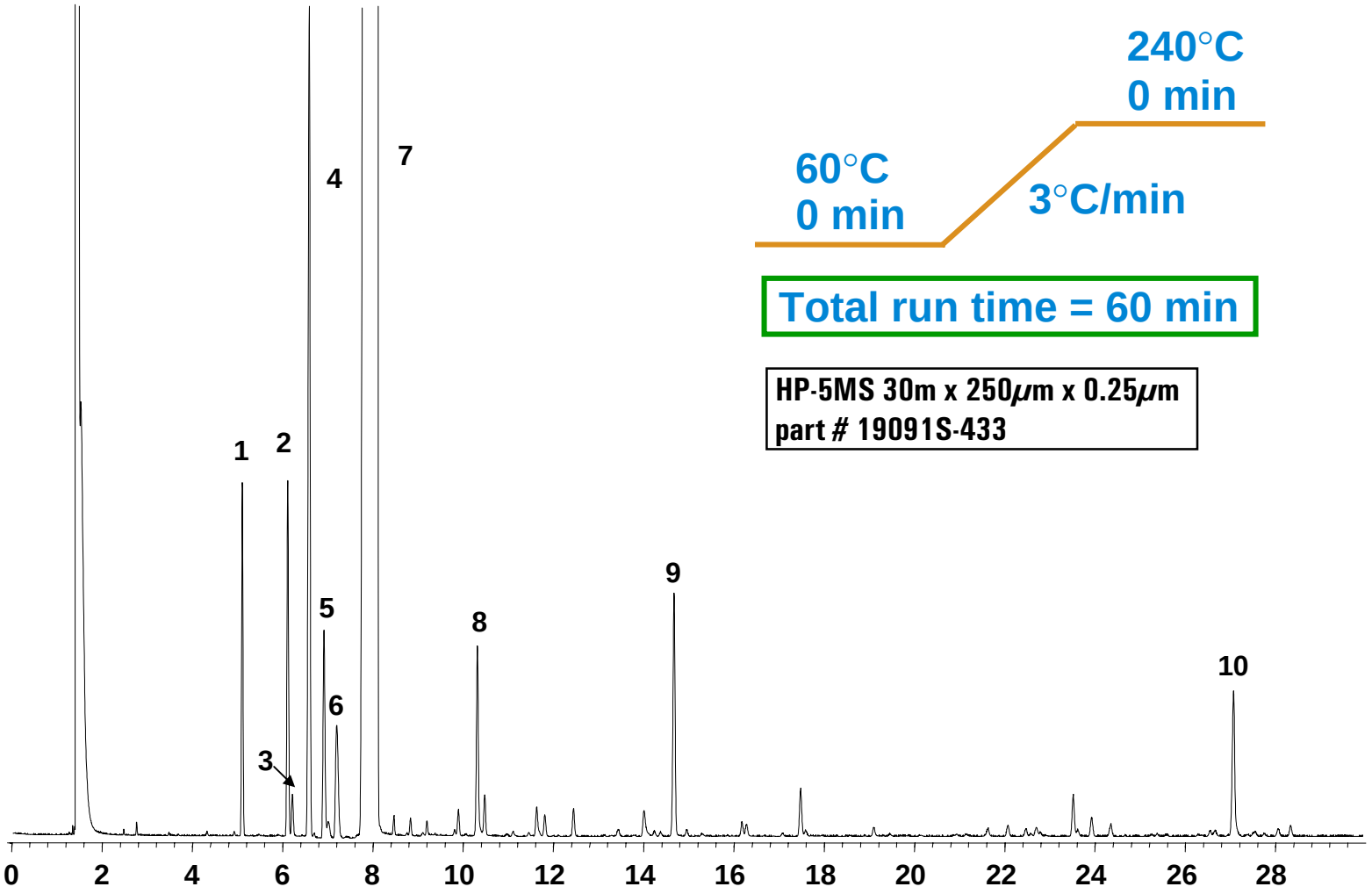
Search Results - Spanish Orange Oil

Peak number	GC-FID t_R (min)	t_R identification	GC-MS t_R (min)	MS + t_R identification
8	40.162	n-undecane cis-3-hexenylpropionate δ-hexalactone 1-methyl-2,3-cyclohexadione linalool methyl benzoate	10.391	linalool
9	48.728	dihydrocarveol methyl salicylate estragole n.decanal octylacetate	14.750	n-decanal
10	71.366	anisylproprionate valencene piperonyl acetate	27.134	valencene

Using the GC/MSD Flavor Databases

- Flavor2.scd and Flavor2.L are copied to the Database folder, usually C:\Database
- The GC/MS system is retention time locked and an RTL method is established
- Samples are run using the RTL method
- Sample data file is Screened using Flavor2.scd
  - Screener report is generated
- Screener Results are reviewed/modified
- Peak spectra can be searched/compared using Flavor2.L

Spanish Orange Oil - RTLocked GC/MSD



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Screener Variables

- The number of probable and possible Hits can be globally changed through these variables
  - Extraction Window for retention time
  - Qualifier Mode, relative or absolute
  - Qualifier %
  - Zero qualifiers, included or excluded
  - Subtraction Mode
- Integration parameters define peak detection

Benefits of Using RTL Databases

- **Fastest identification compounds**
  - **Screen for 409 compounds in < 15 sec**
- **Fastest confirmation of compounds**
  - **Eliminate hits with wrong r.t.**
- **Precise reproducible r.t. on GC and GC/MS**
  - **No need to update calibration tables**
- **Compounds identified by both retention time and spectral information**
- **No additional cost for user-contributed databases**

Flavor Database - RT Order 1 of 6

Ethyl alcohol
Isopropyl formate
Isopropyl alcohol
Isobutyraldehyde
Diacetyl
Butyraldehyde; butanal
Methyl ethyl ketone
Hexane
Ethyl acetate
isobutyl alcohol
3-Methylbutyraldehyde; iso
Butylalcohol
Isopropyl acetate
2-Methylbutyraldehyde; 2-
Propionic acid
1-Penten-3-ol
Methyl isobutyrate
2-Pentanone
Isobutyl formate
Acetyl propionyl
2-Pentanol
n-Valeraldehyde
Pyruvic acid; 2-oxopropan
Heptane
Ethyl propionate
n-Propyl acetate
Ammonium sulfide
Methyl butyrate
Isoamyl alcohol
4-Methyl-2-pentanone
Isobutyric acid
Ethyl isobutyrate
Amyl alcohol
Isobutylacetate
Butyric acid
Methyl-2-methylbutyrate
Isoamyl formate
3,4-Hexanedione
n-Octane
Ethyl butyrate
4-Methyl-3-penten-2-one
Hexenal
2-Methyltetrahydrofuran-3-one
Propyl propionate
n-Butyl acetate
Ethyl lactate
Methylvalerate
2-Methylpyrazine
2-Methyl-2-pentenal
Isovaleric acid
4-Hexene-3-one
5-Methyl-2,3-hexanedione
Ethylcrotonate; ethyl-trans-2
Ethyl-2methylbutyrate
Ethyl isovalerate
trans-2-Hexenal
Furfuryl alcohol
cis-3-Hexenol
2-Hexen-1-ol (trans)
1-Hexanol
Isobutylpropionate
Isoamyl acetate
2-Methylbutylacetate
Valeric acid
Styrene
Isopropyl isovalerate
n-Nonane
2-Heptanol
cis-4-Heptenal
Ethyl valerate
Heptanal
Butyl propionate
trans,trans-2,4-Hexadienal
2-Furyl-methylketone; 2-acet
gamma-Butyrolactone

Flavor Database - RT Order 2 of 6

Isobutyl isobutyrate
Anisole
Methyl caproate; methyl h
Hexyl formate
alpha-Pinene
Ethylacetoacetate
4-Methylpentanoic acid
Propyl isovalerate
Camphene
gamma-Valerolacton
Isobutyl butyrate
trans-2-Heptenal
Benzaldehyde
Heptyl alcohol
Isoamyl propionate
2-Methoxy-3-methylpyrazin
2-Ethylbutyl acetate
sabinene
Methyl-2-furoate
3-(Methylthio)-1-propanol
1-octen-3-ol
Phenol
beta-Pinene
Hexanoic acid
6-Methyl-5-hepten-2-one
2-Octanone
Myrcene
3-Octanol
Furfuryl acetate
Butyl butyrate
n-Decane
3-Hexenoic acid
2-Octanol
2,3,5-Trimethylpyrazine
Octanal
alpha-phellandrene
Isobutyl isovalerate
cis-3-Hexenyl acetate
Ethyl-3-hexenoate
trans,trans-2,4-Heptadienal
delta-3-carene
Hexyl acetate
trans-2-Hexen-1-yl-acetate
2-Methyl-2-pentanoic acid
1,4-Cineole (Isocineole)
trans-2-Hexen-1-yl acetate
alpha-terpinene
p-Methylanisole
2-Acetylpyrazine
Methyl-3-(methylthio)propionate
p-Cymene
2-Ethyl-1-hexanol
Limonene
Eucalyptol
Benzyl alcohol
2-Isobutylthiazole
Isopropyl hexanoate
3,7-Dimethyl-1,3,6-octatriene
Cyclohexyl acetate
n-Butyl-2-methylbutyrate
Phenylacetaldehyde
Ethyl-trans-2-hexenoate
trans-2-Hexenoic acid
Butyl isovalerate
o-Cresol
gamma-Hexalactone
2,6-Dimethyl-5-heptanal
3,4-Dimethyl-1,2-cyclopentad
Isoamylbutyrate
Amyl butyrate
trans-2-octenal
gamma-Terpinene
alpha-Methylbenzylalcohol
Levulinic acid
Ethyl levulinate

Flavor Database - RT Order 3 of 6

Methyl-2-pyrrolyl ketone; 2
Acetophenone
Diethyl malonate
p-Cresol
Linaloloxide (cis, isomer B
m-Cresol
Benzyl formate
Heptanoic acid
Allyl hexanoate
Methyl phenylethyl ether
3,5-Dimethyl-1,2-cyclopent
2,3,5,6-Tetramethylpyrazin
Terpinolene
Linaloxide (trans, isomer A
Guaiacol
2-Nonanone
1-Methyl-2,3-cyclohexadio
delta-Hexalactone
Methyl benzoate
Ethyl heptanoate
n-Undecane
Linalol
Phenethylamine
cis-3-Hexenylpropionate
cis-6-Nonenal

Nonanal
6-Methyl-3,5-heptadien-2-one
3-Acetylpyridine
Isoamyl isovalerate
Methylbutyl-2- isovalerate
Rose oxide (cis); tetrahydro-4-m
Phenethyl alcohol
Heptyl acetate
Fenchyl alcohol
Isophorone
Ethyl-3-hydroxyhexenoate
Methylnicotinate
2-Methylheptanoic acid
Homofuronol; 2-ethyl-4-hydroxy
Isopulegol
Isobutyl caproate; isobutyl hexa
Citronellal
gamma-Heptalactone
trans-2,cis-6-Nonadienal
Neroloxide
Isoborneol (isomer 1)
alpha,alpha-Dimethylphenethyl a
trans-2-Nonenal
3-Phenylpropionaldehyde
2-Methyl-4-propyl-1,3-oxathiane

Menthone
Benzyl acetate
Isoborneol (Isomer 2)
Benzoic acid
p-Methylphenyl acetate
Ethylbenzoate
cis-6-Nonen-1-ol
Nonanol
L-Menthol
Octanoic acid; caprylic acid
Phenethyl formate
4-Carvomenthenol; terpinen
Methyl phenyl acetate
Allyl heptanoate
Diethyl succinate
4’-Methylacetophenone
2,4-Dimethylbenzaldehyde
cis-3-Hexenyl butyrate
alpha-Terpineol
Butyl capronate; butyl hexar
Hexyl butyrate
Methylsalicylate
Dihydrocarveol
cis-4-Decenal
Propyl heptanoate

Flavor Database - RT Order 4 of 6

alpha-Methylbenzylacetate
3,7-Dimethyl-1-octanol
Ethyl octanoate
Estragole
Safranal
n-Dodecane
cis-3-Hexenyl lactate
n-decanal
Octyl acetate
trans,trans-2,4-Nonadiena
Linalyl formate
Phenylacetaldehyde dimet
beta-Cyclocitral
Cyclohexyl butyrate
Cuminaldehyde
Nerol, cis-geraniol
Citronellol
3-Phenyl-1-propanol
cis-3-Hexenyl-2-methyl-bu
Quinoline
cis-3-Hexenyl isovalerate
4-Methyloctanoic acid
Hexyl-trans-2-butenoate
Carvone
Ethylphenyl acetate
Isoamyl hexanoate
p-Anisaldehyde; p-methoxybenz
d-Piperitone
Geraniol
Phenethyl acetate
Phenylacetic acid
gamma-Octalactone
Benzyl propionate
Cinnamaldehyde
Ethyl salicylate
Citral
1-Decanol
Isopropyl phenylacetate
Nonanoic acid
Anisyl alcohol
delta-Octalactone
trans-Anethole
Butyl heptanoate
2-undecanone
Heptyl butyrate
Indole
Thymol
Menthyl acetate; d,L-methyl-2-(m
Ethyl Nonanoate
Benzyl isobutyrate
Carvacrol
Methyl octine carbonate
Geranyl formate
5-Methylquinoxaline
Undecanal
Nonyl acetate
trans,trans-2,4-Decadienal
Citronellic acid; 3,7-dimethy
alpha,alpha-Dimethyl phene
Isobutyl benzoate
Dihydrocarvylacetate
Piperonal; heliotropin
Anisyl formate
Carvyl acetate
Propylphenyl acetate
Methyl anthranilate
3-Phenylpropionic acid
Benzyl butyrate
Terpinyl acetate
2,6-Dimethoxyphenol
Acetanisole
Phenethyl propionate
Triacetin
Benzylidene acetone
Eugenol

Flavor Database - RT Order 5 of 6

Butylbutyryllactate	beta-Caryophyllene	beta-Ionone
gamma-Nonalactone	Anisyl acetate	Veratraldehyde; methyl vanil
Neryl acetate	Linalyl butyrate	Butylated hydroxyanisole
3-Phenylpropyl acetate	Isobutyl salicylate	Dimethyl benzyl carbinyl but
Decanoic acid	Allyl cyclohexyl propionate	Valencene
Dihydrocoumarin	trans-Cinnamic acid	delta-Decalactone
Methyl cinnamate	Geranylaceton (Isomer 1); (E)-6,1	Pentadecane
Dihydrojasmone	Ethyl methylphenylglycidate (iso	Piperonyl acetate
Damascenone	Octyl isovalerate	Anisyl propionate
Geranyl acetate	Phenethyl butyrate	alpha-Irone (isomer 1) (E-); r
Hexyl hexanoate	Citronellyl propionate	Ethyl-3-phenylglycidate
delta-Nonalactone	Cinnamil acetate	Methyl-gamma-ionone (isom
Octyl butyrate	Ethyl-p-anisate	Propenyl guaethol
Benzyl isovalerate	Isoeugenol	Ethyl methylphenylglycidate
Phenethyl isobutyrate	Geranylaceton(isomer 2); (E)-6,1	Citronellyl butyrate
Vanillin	6-Pentyl-alpha-pyrone; 5-hydrox	Nerolidol, (Z-); nerolidol, (cis
Ethyl laurate; ethyl decano	Ethyl cinnamate	alpha-Irone (isomer 2); meth
cis-Jasmone	gamma-Decalactone	nonyl isovalerate
Diphenylether	Ethyl-trans-2, cis-4-decadienoate	Bisabolene
n-Tetradecane	Lauryl alcohol	6-Methylcoumarin
Dimethyl anthranilate	Geranyl propionate	Geranyl butyrate
Lauric aldehyde	5-Hydroxy-2-decanoic acid delta	Nerolidol, (E-); nerolidol, (tra
Decyl acetate	Methyl-gamma-Ionone (isomer 1	Lauric acid
Ethyl anthranilate	Isoamyl octanoate	cis-3-Hexenylbenzoate
beta-Damascone	Isoamyl octanoate	Isoamyl salicylate

Flavor Database - RT Order 6 of 6

gamma-Undecalactone
Cinnamyl isobutyrate
Ethyl laurate
n-Hexadecane
Anisyl butyrate
delta-Undecalactone
Lauryl acetate
Methyljasmonate
Methyl dihydrojasmonate
gamma-Dodecalactone
Farnesol (Z,E-)
delta-Dodecalactone
Farnesol (E,E-)
Amberoxid; dodecahydro-
Benzyl benzoate
Myristic acid
Ethyl myristate
Guaiyl acetate
n-Octadecane
Nootkatone
Isopropyl myristinate
omega-Pentadecalactone
Phenethyloctanoate
Phenethyl phenyl acetate
omega-6-Hexadecalactone
Palmitic acid
Ethyl palmitate
n-Eicosane
Benzyl cinnamate
Ethyl oleate
Stearic acid
ethyloctadecanoate, Ethylsteara
Methional; 3-(methylthio)propion
n-Tetracosane

Agilent Instrumentation Required, GC/MSD

- **Gas Chromatograph**
  - **6890N with autosampler (tray & injector) and split/splitless inlet**
- **Mass Spectrometer**
  - **5973N with EI source**
- **Software**
  - **GC/MSD ChemStation G1701CA version C.00.01 or higher (includes RTL and Screener)**
- **Column**
  - **HP-5MS 30m x 250µm x 0.25µm part # 19091S-433**

Agilent Instrumentation Required, GC/FID

- **Gas Chromatograph**
  - **6890N with autosampler (tray & injector), FID and split/splitless inlet**
- **Software**
  - **GC ChemStation revision A.08.03 or higher**
  - **GC RTL revision A.06.01 or higher**
- **Column**
  - **HP-5 50m x 320µm x 1.05µm part # 19091J-215**

GC/FID Flavor Parameters

GC	Agilent 6890N		
Oven			
Ramp	'C/min	'C	Hold min
Initial		50	0.00
Ramp 1	2	280	0.00
Runtime	115 min		

Inlet	Split/Splitless
Temp	250 'C
Mode	Split
Pressure	12.33 psi (adj to lock)
Split Ratio	25:1 for 5% solution
	100:1 for oils

Column	HP- 5 part # 19091J-215
Mode	Constant pressure
Pressure	12.33 psi
Initial Flow	1.6 mL/min
Outlet Pressure	Ambient

Detector	FID
Temp	250 'C
Hydrogen	40 mL/min
Air	450 mL/min
Nitrogen	45 mL/min
Makeup	

Injector	
Sample Washes	0
Sample Pumps	3
Injection volume	1 uL for 5 % soln.
	0.2 uL for oils
Solv A/B washes	2 each
Viscosity Delay	0
Plunger Speed	Fast

GC/MSD Flavor Parameters

GC	Agilent 6890N		
Oven			
Ramp	'C/min	'C	Hold min
Initial		60	0.00
Ramp 1	3	240	0.00
Runtime	60 min		

Inlet	Split/Splitless
Temp	250 'C
Mode	Split
Pressure	9.43 psi (adj to lock)
Split Ratio	25:1 for 5% solution
	100:1 for oils

Column	HP- 5MS part # 19091S-433
Mode	Constant pressure
Pressure	9.43 psi
Initial Flow	1.2 mL/min
Outlet	MSD
Outlet Pressure	Vacuum

MSD	Agilent 5973N
Solvent Delay	2.0 min
Scan Range	40 to 400
Threshold	150
Sampling	2
Quad Temp	150 'C
Source Temp	230 'C
Transfer Line	280 'C

Injector	
Sample Washes	0
Sample Pumps	3
Injection volume	1 uL for 5 % soln.
	0.2 uL for oils
Solv A/B washes	2 each
Viscosity Delay	0
Plunger Speed	Fast

Recommended Reading

- "Analysis of Essential Oil Compounds Using Retention Time Locked Methods and Retention Time Databases" publication# 5988-6530EN
- Direct your web browser to **www.agilent.com/chem**
- Click on the **Library** link in the left navigation panel
- In the literature search section, enter **5988-6530EN** as the keyword and click the Search button

More Recommended Reading

- Retention Time Locking with the HP G1701BA MSD Productivity ChemStation (5968-3433)
- Efficient Screening for Pesticides and Endocrine Disrupters Using the HP 6890/ 5973 GC/MSD System (5968-4884)
- Retention Time Locking: Concepts and Applications (5966-2469)
- Precise Time-Scaling of Gas Chromatographic Methods Using Method Translation and Retention Time Locking (5967-5820)
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- In the **keyword** field, type in the 8 digit number as it is listed above for the publication you would like to view